ECE 371
Materials and Devices

10/01/19 - Lecture 11

Density of States and Fermi-Dirac Distribution (Occupation Probability)

General Information

- Homework 4 assigned, due Tuesday 10/15
- Please do not plot by hand – use Matlab or Excel
- Midterm solutions posted
- Reading for next time: 4.1, 4.2

Carrier Density and Density of States

- Goal: determine the electron (n) and hole (p) densities ($\#/cm^3$) in the semiconductor

$$\boxed{n = \int g_c(E) f_F(E)\, dE}$$

Density of allowed states per unit volume per unit energy

Probability that an allowed state is occupied by an electron

- The density of states (DOS) describes the density of allowed states per unit volume per unit energy (g(E))
- Electron and holes are called “carriers”
- First we will calculate the DOS portion of the carrier density

Density of States (DOS)

- To determine the 3D DOS in k-space:

1. Calculate the number of states ($N_s(k)$) as a function of k contained within the sphere bounded by $k^2 = k_x^2 + k_y^2 + k_z^2$ by taking the volume of the sphere in k-space ($V_{sphere} = (4/3)\pi k^3$) divided by unit volume of one state in k-space ($V_{unit-k} = (\pi/a)^3$)
2. Multiply by 2 for spin degeneracy and divide by 8 to keep only positive k-values
3. Using the parabolic approximation for a free electron, convert $N_s(k)$ to $N_s(E)$
4. Divide by a unit volume in real space $V_{unit} = a^3$
5. Differentiate with respect to E, dN_s/E, to get the DOS

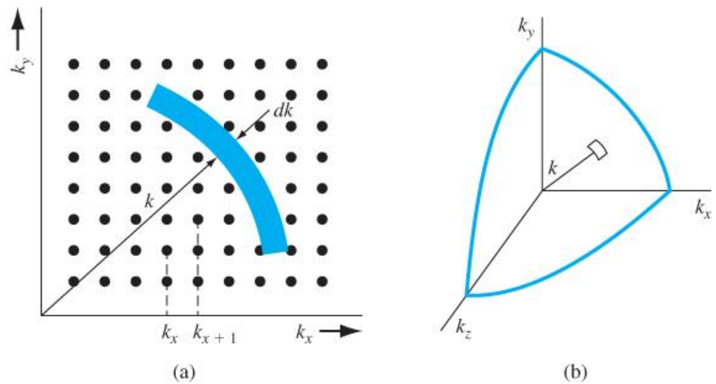


Figure 3.26 | (a) A two-dimensional array of allowed quantum states in k space. (b) The positive one-eighth of the spherical k space.

$$DOS = \frac{1}{V_{unit}} \frac{dN_s}{dE}$$

V_{unit} = unit volume
N_s = # of states
E = energy

Semiconductor Density of States (3D)

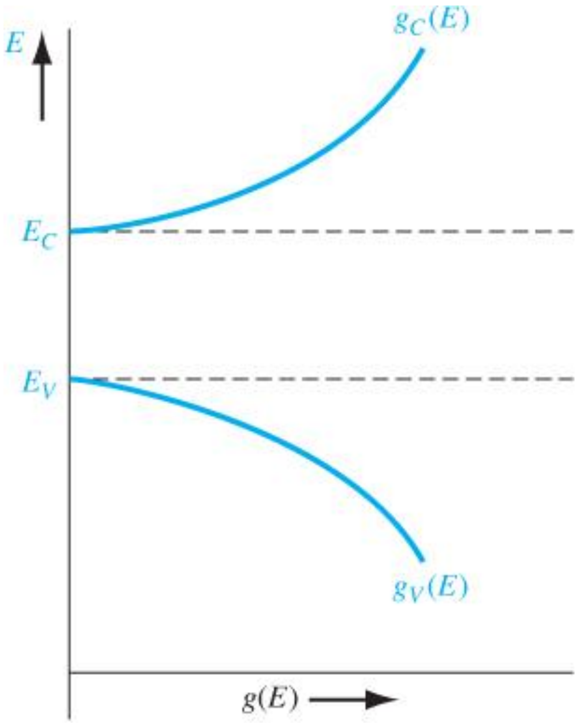


Figure 3.27 | The density of energy states in the conduction band and the density of energy states in the valence band as a function of energy.

Conduction band DOS:

$$\boxed{g_c(E) = \frac{4\pi}{h^3}[2m_n^*]^{3/2}(E - E_c)^{1/2}}$$

Valence band DOS:

$$\boxed{g_v(E) = \frac{4\pi}{h^3}\left[2m_p^*\right]^{3/2}(E_v - E)^{1/2}}$$

- Parabolic approximation
- Fewer states at lower energies
- No states in the forbidden gap
- In general, $g_c(E)$ and $g_v(E)$ are different
- 3D DOS is also called “bulk” DOS

Density of States (Lower Dimensions)

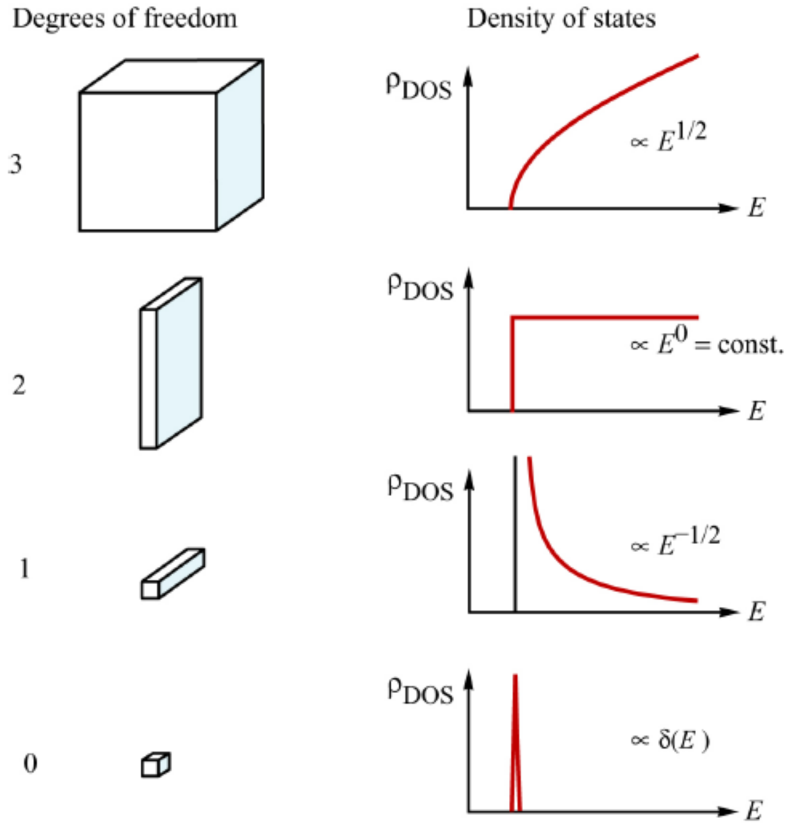


Fig. 12.7. Electronic density of states of semiconductors with 3, 2, 1, and 0 degrees of freedom for electron propagation. Systems with 2, 1, and 0 degrees of freedom are referred to as quantum wells, quantum wires, and quantum boxes, respectively.

Common Statistical Distributions

- Statistical mechanics: used to describe the behavior of large numbers of particles
  - Maxwell-Boltzmann:
    - Any number of particles in each state
    - Distinguishable and non-interacting particles
    - Gas molecules in a container
  - Bose-Einstein:
    - Any number of particles in each state
    - Indistinguishable and non-interacting particles
    - Photons or other bosons (integer spin) — integers
  - Fermi-Dirac:
    - Only one particle per quantum state (Pauli exclusion)
    - Indistinguishable and non-interacting particles
    - Electrons and other Fermions (non-integer spin) — $\frac{1}{2}$ or $-\frac{1}{2}$

only ones we'll study

$$W_i = \binom{N_i}{g_i} = \frac{g_i!}{N_i!\,(g_i - N_i)!}$$ (n choose k)

$$\text{total Ways} = \prod_{i=1}^{n} \frac{g_i!}{N_i!\,(g_i - N_i)!}$$

Fermi-Dirac Distribution

Describes the probability that an available state is filled at a given energy and temperature

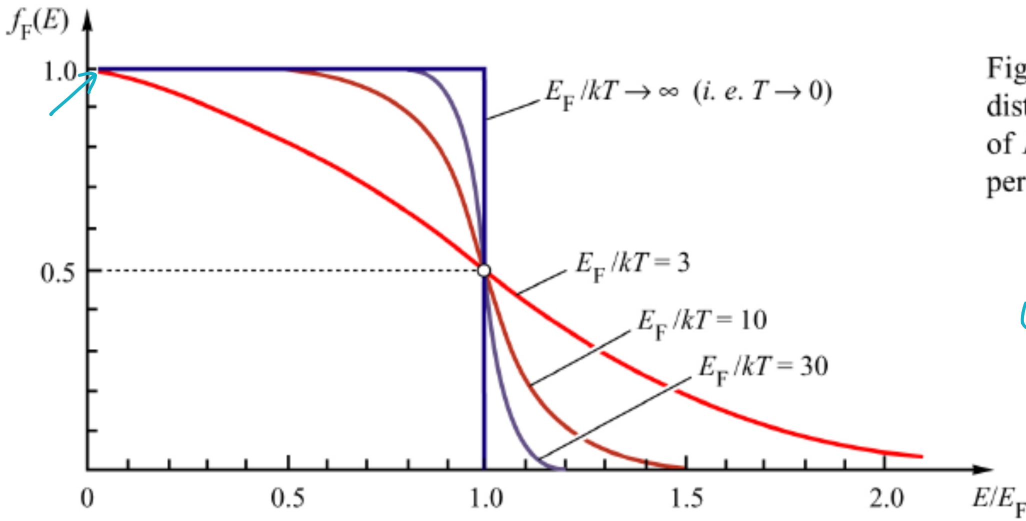


Fig. 13.4. Fermi–Dirac distribution as a function of E/E_F for different temperatures.

$0 \leq f_F(E) \leq 1$

(probab. density)

Fermi-Dirac = Most probable distribution

$$\boxed{f_F(E) = \frac{1}{e^{(E-E_F)/kT} + 1}}$$

fermi energy (fermi level)

*E_F is the Fermi energy

Fermi-Dirac Distribution (T = 0K)

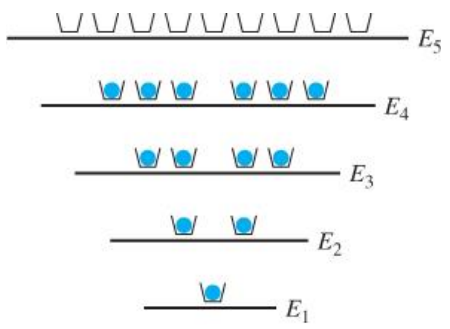


Figure 3.30 | Discrete energy states and quantum states for a particular system at $T = 0$ K.

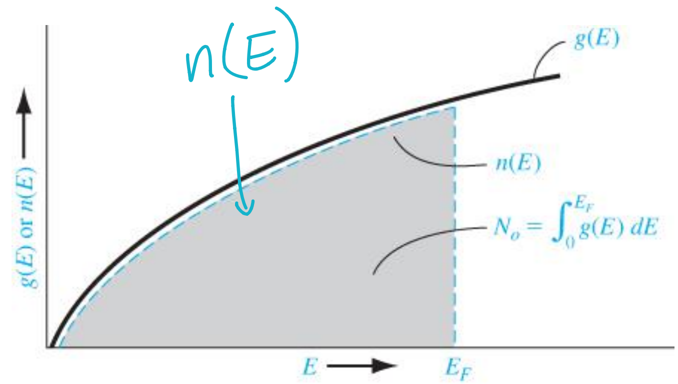


Figure 3.31 | Density of quantum states and electrons in a continuous energy system at $T = 0$ K.

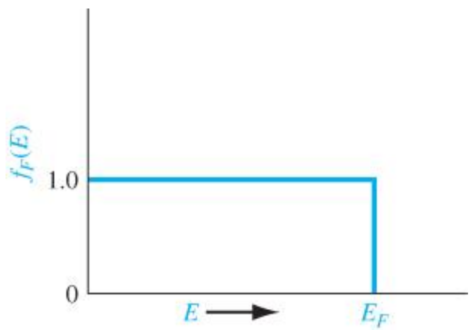


Figure 3.29 | The Fermi probability function versus energy for $T = 0$ K.

- Electrons occupy the lowest available energy states
- All electrons have energies below E_F

At $T = 0K$

1. $E < E_F \quad e^{\left(\frac{E-E_f}{0}\right)} \longrightarrow e^{-\infty} \longrightarrow f_F(E) = 1$

   always filled

2. $E > E_F \quad \longrightarrow e^{\infty} \longrightarrow f_F(E) = 0$

   always empty

3. $E = E_F \quad \longrightarrow f_F(E) = \frac{1}{2}$

Fermi-Dirac Distribution (T > 0K)

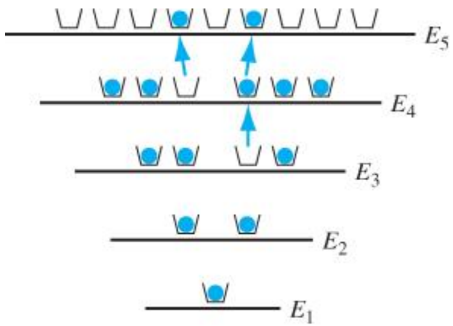


Figure 3.32 | Discrete energy states and quantum states for the same system shown in Figure 3.30 for $T > 0$ K.

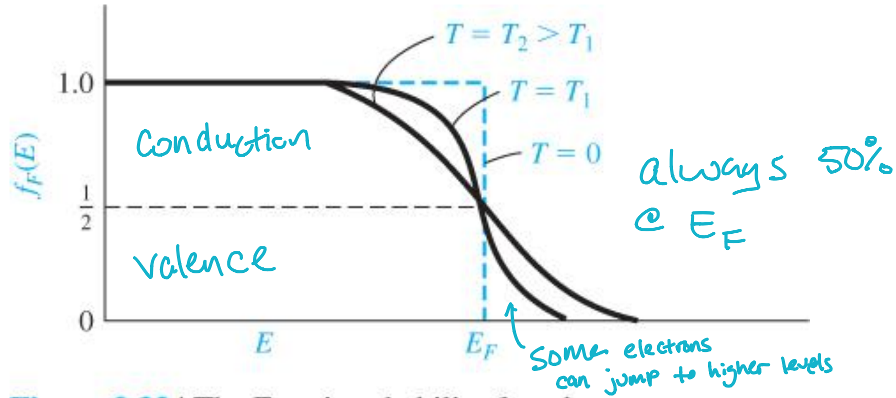


Figure 3.33 | The Fermi probability function versus energy for different temperatures.

- At T > 0K, some electrons have enough energy to jump to higher energy levels
- Higher temperatures result in a smeared distribution around the Fermi energy

Exercise Problems

EXERCISE PROBLEM

Ex3.6 Assume the Fermi energy level is 0.30 eV below the conduction band energy E_c. Assume $T = 300$ K. (a) Determine the probability of a state being occupied by an electron at $E = E_c + kT/4$. (b) Repeat part (a) for an energy state at $E = E_c + kT$.

[Ans. (a) 7.26×10^{-6}; (b) 3.43×10^{-6}]

EXERCISE PROBLEM

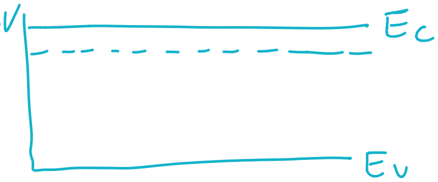
Ex 3.7 Assume that E_F is 0.3 eV below E_c. Determine the temperature at which the probability of an electron occupying an energy state at $E = (E_c + 0.025)$ eV is 8×10^{-6}.

(Ans. $T = 321$ K)

$$E = E_c + \frac{kT}{4} = \cancel{E_c + 1.035}$$

$$kT = 26mV$$

$$E_F = E_c - 0.3eV$$



$$\boxed{f_F(E) = \frac{1}{e^{(E-E_F)/kT} + 1}}$$

$$f_F(E) = \frac{1}{e^{0.3065/kT} + 1}$$

$$E - E_F$$

$$\cancel{E_c} - \frac{kT}{4} - \cancel{E_c} + 0.3eV = \frac{0.026}{4}eV + 0.3eV = 0.3065eV$$

$$f_F(E) = \frac{1}{e^{0.3065/kT} + 1} = 7.59 \times 10^{-6}$$

Probability of Non-Occupation

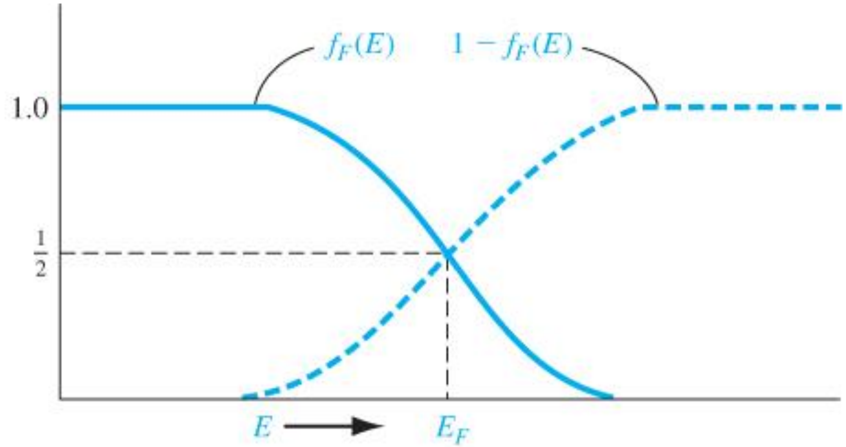


Figure 3.34 | The probability of a state being occupied, $f_F(E)$, and the probability of a state being empty, $1 - f_F(E)$.

- The probability of non-occupation (i.e. – of finding an empty state) is $1 - f_F(E)$
- Applicable to holes → only in valence band!!

Holes concentration

$$p = \int g_v(E)\,(1 - f_F(E))\,dE$$

Maxwell – Boltzmann Approximation

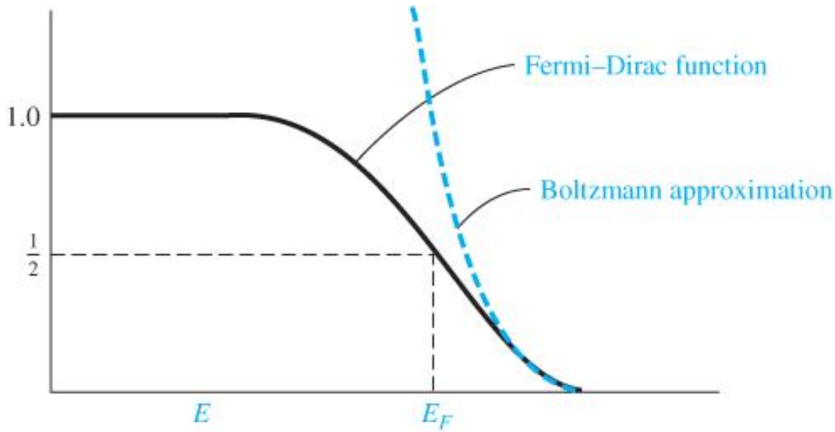


Figure 3.35 | The Fermi–Dirac probability function and the Maxwell–Boltzmann approximation.

$$\boxed{f_F(E) \approx e^{-(E-E_F)/kT}}$$

valid when $E - E_F \gg kT$

$E - E_F > 3kT$

gives 5% error

- Approximation to the Fermi-Dirac distribution when the energy of interest (E) is far above the Fermi energy
- Useful to simplify expressions for carrier density

find lowest temp to get certain Temp

- Applicable to LEDs under low-level injection and some electronic devices. Not typically applicable to diode lasers.

Carrier Density vs. Energy

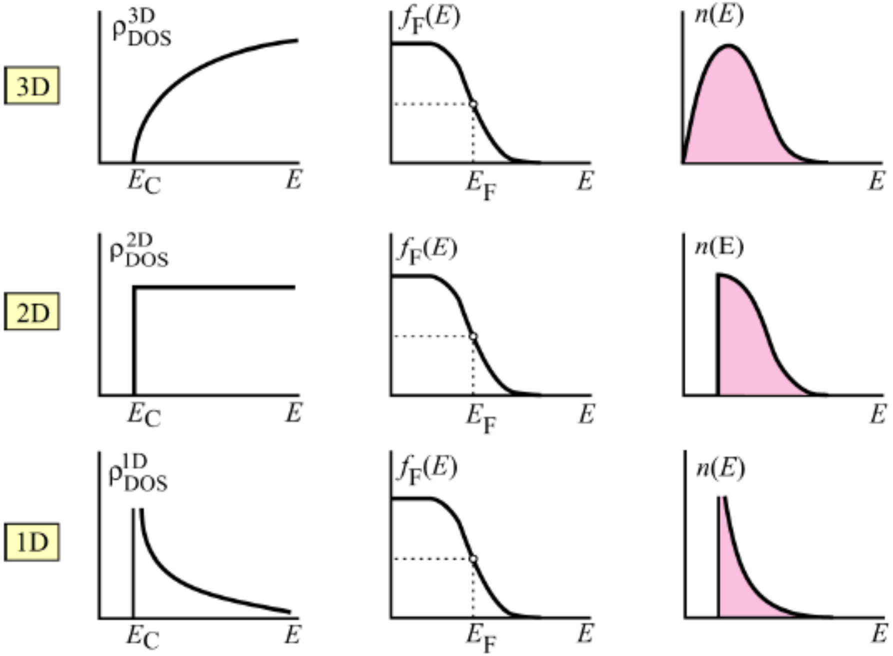


Fig. 13.5. Density of states (ρ_{DOS}), Fermi-Dirac distribution function (f_F) and carrier concentration (n) as a function of energy for a 3D, 2D, and 1D system. The shaded areas represent the total carrier concentration in the conduction band.

electron density

$$\boxed{n = \int g_c(E)\, f_F(E)\, dE}$$

hole density

$$\boxed{p = \int g_v(E)[1 - f_F(E)]\, dE}$$

Example

TEST YOUR UNDERSTANDING

TYU 3.5 Assume that the Fermi energy level is 0.35 eV above the valence band energy. Let $T = 300$ K. (a) Determine the probability of a state being empty of an electron at $E = E_v - kT/2$. (b) Repeat part (a) for an energy state at $E = E_v - 3kT/2$.
[Ans. (a) 8.20×10^{-7}; (b) 3.02×10^{-7}]